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# Computation of the b-Quark Mass with Perturbative Matching at the Next-to-Next-to-Leading Order

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## Abstract

We compute the two-loop term in the perturbation series for the quark-mass in the lattice Heavy Quark Effective Theory (HQET). This is an ingredient in the matching factor required to obtain the  $b$ -quark mass from lattice simulations of the HQET. Combining our calculation with numerical results from the APE collaboration, we find, at two-loop order,  $\overline{m}_b \equiv m_b^{\overline{MS}}(m_b^{\overline{MS}}) = 4.41 \pm 0.05 \pm 0.10 \text{ GeV}$ . It was expected that the two-loop term would have a significant effect, and this is indeed what we find. Depending on the choice of “reasonable” coupling constant in the one-loop estimates, the result for  $\overline{m}_b$  can change by several hundred MeV when the two-loop terms are included.

# 1 Introduction

In this paper we evaluate the two-loop perturbative matching factor required to obtain the mass of a heavy quark from lattice simulations of the Heavy Quark Effective Theory (i.e. from simulations of static heavy quarks). This is the next-to-next-to-leading-order (NNLO) term in the matching factor. We combine this matching factor with numerical results from simulations to obtain:

$$\boxed{\overline{m}_b = 4.41 \pm 0.05 \pm 0.10 \text{ GeV}} \quad (1)$$

where

$$\overline{m}_b \equiv m_b^{\overline{\text{MS}}}(m_b^{\overline{\text{MS}}}) \text{ ,} \quad (2)$$

at NNLO. The first error in eq. (1) is due to the uncertainties in the values of the lattice spacing, in the value of the strong coupling constant and in the numerical evaluation of the functional integral. The second error is an estimate of the uncertainties due to our ignorance of 3-loop and higher order perturbative terms.

For the Lagrangian of the HQET we take:

$$\mathcal{L}_{\text{HQET}} = \bar{h} D_4 \frac{1 + \gamma^4}{2} h \text{ ,} \quad (3)$$

where  $h$  is the field of the heavy quark, and we use the following definition of the covariant derivative  $D$ :

$$D_\mu h(x) = U_\mu(x) h(x + \hat{\mu}) - h(x) \text{ ,} \quad (4)$$

where  $x + \hat{\mu}$  is the neighbouring point to  $x$  in the  $\mu$ -direction.  $U_\mu(x)$  is the link variable from  $x$  to  $x + \hat{\mu}$ . For the light-quark action we take an “improved” generalisation of the Wilson action. For each quark flavour the action is:

$$S_q = S_W + c_{\text{SW}} S_{\text{SW}} \text{ ,} \quad (5)$$

where  $S_W$  is the Wilson fermion action:

$$S_W = \sum_x \left\{ -\frac{1}{2} \sum_\mu \left[ \bar{\psi}(x)(1 - \gamma_\mu)U_\mu(x)\psi(x + \hat{\mu}) + \bar{\psi}(x + \hat{\mu})(1 + \gamma_\mu)U_\mu^\dagger(x)\psi(x) \right] \right. \\ \left. + \bar{\psi}(x)(m_0 + 4)\psi(x) \right\} \text{ ,} \quad (6)$$

and  $S_{\text{SW}}$  is the Sheikholeslami-Wohlert (or “clover”) action [1]

$$S_{\text{SW}} = -\frac{i}{4} \sum_{x,\mu,\nu} \left[ \bar{\psi}(x)\sigma_{\mu\nu}F_{\mu\nu}(x)\psi(x) \right] \text{ .} \quad (7)$$



Figure 1: (a) A one-loop diagram and (b) a two-loop diagram contributing to  $\delta m$ . The solid lines represent static heavy quarks.

$F_{\mu\nu}$  is the lattice expression of the field-strength tensor obtained by averaging the four plaquettes lying in the  $(\mu, \nu)$  plane and stemming from the point  $x$ . The coefficient  $c_{\text{SW}}$  is equal to 1 at tree-level (with  $c_{\text{SW}} = 1$  and using appropriate operators the discretisation errors in physical quantities are reduced from  $O(a)$  for the Wilson action to  $O(\alpha_s a)$ ). Recently much effort has been devoted to fixing  $c_{\text{SW}}$  non-perturbatively in such a way that the errors are reduced to ones of  $O(a^2)$  [2]. For the perturbative calculations in this paper we will keep  $c_{\text{SW}}$  and  $N_f$ , the number of light-quark flavours as free parameters <sup>1</sup>.

The starting point for our evaluation of the heavy quark mass is the computation of the correlation functions of the time-component of two axial currents:

$$C(t) = \sum_{\vec{x}} \langle 0 | A_4(x) A_4^\dagger(0) | 0 \rangle \quad (8)$$

$$\simeq Z^2 \exp(-\mathcal{E}t) , \quad (9)$$

where we have assumed that  $t$  is positive and sufficiently large so that we can neglect the contributions from excited states. The current takes the form <sup>2</sup>  $A_4(x) = \bar{h}(x) \gamma_4 \gamma_5 q(x)$  (the factor of  $\gamma_4$  can be replaced by the Identity since it is adjacent to the heavy quark field). By fitting the correlator  $C(t)$  as a function of  $t$ , both the prefactor  $Z$  and the exponent  $\mathcal{E}$  can be determined. From  $Z$  we can obtain the decay constant of a heavy pseudoscalar meson in the static limit, whereas from  $\mathcal{E}$  we obtain  $\overline{m}_b$  [3]. Matching QCD and the Lattice HQET one finds that [3]:

$$m_b^{\text{pole}} = M_B - \mathcal{E} + \delta m , \quad (10)$$

where  $m_b^{\text{pole}}$  is the “pole” mass of the  $b$ -quark,  $M_B$  is the physical mass of the  $B$ -meson and  $\delta m$  is the mass generated in the static theory, eq. (3), in perturbation theory ( $a\delta m = \alpha_s X_0 + \alpha_s^2 X_1$ , where the coefficient  $X_1$  depends on the choice of coupling constant,  $\alpha_s$ , used in the perturbative expansion). Even though there is no explicit mass-term in the bare action of eq. (3), Feynman diagrams, such as those in fig. 1, generate such a term which is proportional to  $1/a$ , where  $a$  is the lattice spacing. Once  $m_b^{\text{pole}}$  is known, then

<sup>1</sup>The results are also presented for an arbitrary number of colours,  $N$ .

<sup>2</sup>In practice it is generally advantageous to use “smeared” interpolating operators in order to enhance the overlap with the ground state.

any physical, short-distance, quark mass can be determined using continuum perturbation theory, e.g.

$$\overline{m}_b = (M_B - \mathcal{E} + \delta m) \left[ 1 - \frac{4}{3} \left( \frac{\alpha_s(\overline{m}_b)}{\pi} \right) - (11.66 - 1.04 N_f) \left( \frac{\alpha_s(\overline{m}_b)}{\pi} \right)^2 + O(\alpha_s^3(\overline{m}_b)) \right], \quad (11)$$

where  $N_f$  is the number of light-quark flavours and  $\alpha_s$  is defined in the  $\overline{\text{MS}}$  renormalization scheme. The term in square brackets in eq. (11) is the perturbative expansion of the factor which relates the pole mass to the  $\overline{\text{MS}}$  one [4]. *The main aim of this paper is to calculate  $\delta m$  to two-loop order.* Using the  $\overline{\text{MS}}$  coupling  $\alpha_s(\overline{m}_b)$  as the expansion parameter we find

$$a \delta m = 2.1173 \alpha_s(\overline{m}_b) + \{ (3.707 - 0.225 N_f) \ln(\overline{m}_b a) - 1.306 - N_f (0.104 + 0.100 c_{\text{SW}} - 0.403 c_{\text{SW}}^2) \} \alpha_s^2(\overline{m}_b). \quad (12)$$

Consider eqs. (10), (11) and (12). Neither the perturbation series for  $\delta m$  nor that relating  $m_b^{\text{pole}}$  and  $\overline{m}_b$  in the square brackets in eq. (11) is Borel summable and both contain renormalon ambiguities. In each case the leading ambiguity is of  $O(\Lambda_{\text{QCD}})$ . Since  $m_b^{\text{pole}}$  is not a physical quantity, the presence of a renormalon on the right-hand side of eq. (10) is not inconsistent.  $\overline{m}_b$ , however, is a physical quantity, and the leading renormalon ambiguity cancels when the two perturbation series in eq. (11) are combined [5, 6, 7]<sup>3</sup>. The remaining renormalon ambiguity is of  $O(\Lambda_{\text{QCD}}^2/\overline{m}_b)$  which is beyond the precision we are considering in this paper. Related to the problem of renormalons is that of power divergences (i.e. the terms which behave as powers of  $a^{-1}$ ).  $\delta m$  diverges linearly with the inverse lattice spacing, cancelling the linear divergence in  $\mathcal{E}$  (this cancellation is necessarily only partial since we truncate the perturbation series for  $\delta m$  at a finite order of perturbation theory). Thus by computing  $\mathcal{E}$  numerically, and calculating  $\delta m$  and the relation between the pole-mass and  $\overline{m}_b$  in perturbation theory (this relation is known to two-loop order [4]),  $\overline{m}_b$  can be obtained. It is free of power divergences and renormalon ambiguities.

Although we do not present the discussion explicitly in the formalism of an Operator Product Expansion, the calculation of the quark mass here is an example of the evaluation of a power correction. To lowest order in the heavy quark expansion we can take  $m_b = M_B$ , and we are evaluating the first power corrections to this (i.e. the correction of  $O(\Lambda_{\text{QCD}})$  relative to the leading term). In ref. [7] we argued that the evaluation of power corrections is difficult, requiring high-orders of perturbation theory in order to subtract the power divergences to sufficient precision. To illustrate this point for the heavy-quark mass, we show in subsection 3.1.3 that the one-loop result changes by several hundred MeV depending on which “reasonable” coupling constant is used in the one-loop result (specifically we use the  $\overline{\text{MS}}$  coupling at an average momentum  $q^*$ , the  $V$  coupling defined from the potential also at the scale  $q^*$  and a boosted lattice coupling constant). The two-loop calculation described in this paper reduces this uncertainty to 100 MeV or less.

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<sup>3</sup>In order for this cancellation to be manifest, a single coupling constant for both perturbation series must be used (we use  $\alpha_s(\overline{m}_b)$ ).

In the present calculation the ultra-violet divergences are linear in the inverse lattice spacing. For other physical quantities for which the power divergences are quadratic (or even higher order) it is even more difficult to control the perturbative corrections [7].

The plan for the remainder of this paper is as follows. In the next section we present the outline of the perturbative calculation of  $\delta m$  up to two-loop order. In an attempt to make the steps of the calculation clearer, we have relegated the technical details to a (rather long) appendix. In section 3 we use our perturbative results in order to determine the mass of the  $b$ -quark from values of  $\mathcal{E}$  obtained in numerical simulations. Finally in section 4 we present our conclusions.

## 2 Calculation of $\delta m$ to Two-Loop Order

In this section we outline the evaluation of  $\delta m$  up to two-loop order in perturbation theory. Instead of evaluating self-energy diagrams, such as those in fig. 1, directly, we exploit the fact that two-loop perturbative results for rectangular Wilson loops have already been presented [8, 9]. We therefore determine  $\delta m$  from the exponential behaviour of large Wilson loops as we now explain.

Consider a Wilson loop ( $W(R, T)$ ) in the  $\mu$ - $\nu$  plane, of length  $R$  and  $T$  in the  $\mu$  and  $\nu$  directions respectively. Since, *in perturbation theory*, the potential between static-quarks falls like  $1/r$  with their separation  $r$ , the expectation value of large Wilson loops decrease exponentially with the perimeter of the loops, specifically

$$\langle W(R, T) \rangle \sim \exp(-2\delta m(R + T)) . \quad (13)$$

Hence the perimeter term in  $\log(\langle W(R, T) \rangle)$  is simply  $-2\delta m(R + T)$ .

Following ref. [8] we define the first two coefficients of the perturbative expansion for  $\langle W(R, T) \rangle$  as follows:

$$\langle W(R, T) \rangle = 1 - g^2 W_2(R, T) - g^4 W_4(R, T) + O(g^6) , \quad (14)$$

where  $g$  is the bare lattice coupling constant. By using eq. (13) we obtain the perturbative expansion for  $\delta m$  in terms of these coefficients,

$$\delta m = \frac{1}{2(R + T)} \left[ g^2 W_2(R, T) + g^4 \left( W_4(R, T) + \frac{1}{2} W_2^2(R, T) \right) \right] . \quad (15)$$

We now evaluate  $W_2$  and  $W_4$ , only keeping terms which grow at least linearly with the dimensions of the Wilson loop.

### 2.1 Evaluation of $W_2(R, T)$

In ref. [8] we find the following integral representation of  $W_2$  for an  $SU(N)$ -gauge theory:

$$W_2(R, T) = \frac{(N^2 - 1)}{N} \int_{-\pi}^{\pi} \frac{d^4 p}{(2\pi)^4} \frac{\sin^2(\frac{1}{2} p_\nu T) \sin^2(\frac{1}{2} p_\mu R)}{D(p)} \left\{ \frac{1}{\sin^2(\frac{1}{2} p_\mu)} + \frac{1}{\sin^2(\frac{1}{2} p_\nu)} \right\} , \quad (16)$$

where

$$D(p) = 4 \sum_{\lambda=1}^4 \sin^2(\frac{1}{2}p_\lambda) . \quad (17)$$

Consider the first term in the integrand in eq. (16), i.e. the term containing a factor of  $1/\sin^2(\frac{1}{2}p_\mu)$ . By inspection (i.e. by using power counting) it can be seen that the region of small  $p_\mu$  gives a contribution proportional to  $R$  (and similarly the second term gives a contribution proportional to  $T$ ). By changing variables from  $p_\mu$  to  $z = \exp(ip_\mu)$  (so that the contour of integration in  $z$  is the unit circle), and studying the singularities of the integrand in  $z$ , the integration over  $z$  can be performed. In this way one obtains

$$W_2(R, T) \equiv \frac{(N^2 - 1)}{4N} \overline{W}_2(R, T) = \frac{(N^2 - 1)}{4N} \{ (R + T) X - Y(R) - Y(T) \} , \quad (18)$$

where  $X$  and  $Y$  are three-dimensional integrals defined in eqs. (A.1) and (A.4) of the appendix.  $X$  is a finite integral, whereas  $Y(R)$  grows logarithmically with  $R$ .  $\delta m$  at one-loop level is given by the term in the perimeter which is proportional to  $X$ . We will, however, require the terms proportional to  $Y(R) + Y(T)$  when we evaluate  $\delta m$  at two-loops (see eq. (15)). Equation (18) implies that

$$\delta m = \frac{N^2 - 1}{8N} X g^2 + O(g^4) , \quad (19)$$

which is the well known one-loop result.

## 2.2 Evaluation of $W_4(\mathbf{R}, \mathbf{T})$

The evaluation of  $W_4(R, T)$  is the main calculation of this paper, and we describe this calculation in some detail in the Appendix. We write

$$W_4(R, T) = W_4^{\text{gluon}}(R, T) + W_4^{\text{fermion}}(R, T) , \quad (20)$$

where  $W_4^{\text{gluon}}(R, T)$  is the contribution from diagrams in the pure-gauge theory and  $W_4^{\text{fermion}}(R, T)$  is that from diagrams containing light-quark loops. The purely gluonic contribution is given in eq. (A.50)

$$\begin{aligned} W_4^{\text{gluon}}(R, T) = & -\frac{(N^2 - 1)^2}{32N^2} X^2 (R + T)^2 + \frac{(N^2 - 1)^2}{16N^2} X (Y(R) + Y(T)) (R + T) \\ & + \frac{(N^2 - 1)}{192} \{ 3X^2 - 2XL + 12W \} (R + T) \\ & + \frac{(N^2 - 1)}{96} \left\{ 3V_1 + 6V_2 + 7LX - \frac{5}{4}X \right\} (R + T) + \left\{ \frac{(N^2 - 1)(2N^2 - 3)}{96N^2} X \right\} (R + T) , \end{aligned} \quad (21)$$

Integral	Defined in eq.	Value
$X$	(A.1)	0.50546
$L$	(A.3)	0.30987
$W$	(A.6)	$1.313(3) \cdot 10^{-2}$
$V_1$	(A.7)	$7.008(5) \cdot 10^{-2}$
$V_2$	(A.9)	$-2.130(1) \cdot 10^{-2}$
$V_W$	(A.14)	$-2.145(1) \cdot 10^{-2}$
$V_{SW}^a$	(A.15)	$2.63(2) \cdot 10^{-3}$
$V_{SW}^b$	(A.15)	$-2.974(1) \cdot 10^{-2}$

Table 1: Values of the integrals used in the evaluation of  $\delta m$  to two-loops in perturbation theory.

and the contribution from graphs containing light-quark loops is given in eq. (A.52)

$$W_4^{\text{fermion}}(R, T) = \frac{(N^2 - 1)N_f}{16N} (R + T) (V_W + V_{SW}) , \quad (22)$$

where  $N_f$  is the number of active light-quark flavours. The integrals  $X, L, Y, W, V_{1,2}, V_W$  and  $V_{SW}$  in these expressions are defined and evaluated in section A.1 of the appendix.  $V_{SW}$  is the contribution from the improvement term in the fermionic action and we write it as  $V_{SW} = V_{SW}^a c_{SW} + V_{SW}^b c_{SW}^2$ . With the exception of  $Y(R)$ , which depends logarithmically on  $R$  and cancels out of the expression for  $\delta m$ , we present the numerical values of these integrals in table 1.

## 2.3 The Perturbation Series for $\delta m$

Having determined the relevant terms in  $W_2(R, T)$  and  $W_4(R, T)$  we can readily obtain the perturbation series for  $\delta m$  using eq. (15). At one-loop order, the result is presented in eq. (19) which, setting the number of colours  $N$  equal to 3, we rewrite as:

$$a \delta m \simeq 2.1173 \alpha_0 + O(\alpha_0^2) , \quad (23)$$

where the subscript 0 on  $\alpha_0$  reminds us that the expansion is in terms of the bare coupling constant in the lattice theory.

The two-loop contribution to  $\delta m$  is proportional to  $W_4(R, T) + \frac{1}{2}W_2^2(R, T)$  (see eq. (15)):

$$W_4(R, T) + \frac{1}{2}W_2^2(R, T) = (R + T) \frac{(N^2 - 1)}{192} \left\{ 3X^2 + 12W + 6V_1 + 12V_2 + \right. \\ \left. 12LX + \frac{3(N^2 - 4)}{2N^2} X + \frac{12N_f}{N} (V_W + V_{SW}) \right\} . \quad (24)$$

The terms quadratic in  $R$  and  $T$  explicitly cancel in the combination  $W_4 + \frac{1}{2}W_2^2$ , as do those proportional to the integrals  $Y(R)$  and  $Y(T)$  as they must. This is an important consistency check of our calculations. All the integrals on the right-hand side of eq. (24) are finite and independent of  $R$  and  $T$ . Substituting  $N = 3$  and the numerical values of the integrals (see the appendix) in the right-hand side of eq. (24), we obtain <sup>4</sup>

$$W_4(R, T) + \frac{1}{2}W_2^2(R, T) = (R + T) \{0.14124 + N_f(-0.00358 + 0.00044 c_{\text{SW}} - 0.00496 c_{\text{SW}}^2)\}. \quad (25)$$

We thus arrive at the two-loop expression for  $\delta m$ :

$$a \delta m \simeq 2.1173 \alpha_0 + \{11.152 + N_f(-0.282 + 0.035 c_{\text{SW}} - 0.391 c_{\text{SW}}^2)\} \alpha_0^2 + O(\alpha_0^3). \quad (26)$$

Eq. (26) is the main result of this paper. In the following section we will exploit this result to extract the mass of the  $b$ -quark from the values of  $\mathcal{E}$  computed in lattice simulations.

### 3 Lattice Computation of $m_b$

In this section we discuss the evaluation of the heavy quark mass, from lattice computations of  $\mathcal{E}$  using the two-loop result for  $\delta m$  in eq. (26). For illustration we will determine the  $\overline{\text{MS}}$ -mass,  $\overline{m}_b$ , defined in eq. (2), from which any other short-distance definition of the heavy-quark mass can be obtained using continuum perturbation theory.

As discussed in the introduction, the relation between  $\overline{m}_b$  and  $\mathcal{E}$  is:

$$\overline{m}_b = (M_B - \mathcal{E} + \delta m) \left[ 1 - \frac{4}{3} \left( \frac{\alpha_s(\overline{m}_b)}{\pi} \right) - (11.66 - 1.04 N_f) \left( \frac{\alpha_s(\overline{m}_b)}{\pi} \right)^2 \right], \quad (27)$$

where  $N_f$  is the number of light-quark flavours and  $\alpha_s$  is defined in the  $\overline{\text{MS}}$  renormalization scheme. In eq. (11),  $M_B = 5.279$  GeV is the physical mass of the  $B$ -meson,  $\mathcal{E}$  is computed in lattice simulations and the remaining terms are calculated in perturbation theory. The term in square brackets in eq. (11) is the perturbation expansion of the factor which relates the pole mass to the  $\overline{\text{MS}}$  one [4].

The two-loop expression for  $\delta m$  in eq. (26) is given in terms of  $\alpha_0$ , the bare coupling constant in the lattice theory. In order to achieve the explicit cancellation of renormalon singularities the same coupling constant needs to be used in the expansion of  $\delta m$  and in the relation between the pole mass and the  $\overline{\text{MS}}$  mass (i.e. in the expression in square parentheses in eq. (11)). The relation between the  $\overline{\text{MS}}$  coupling  $\alpha_s$  and the lattice coupling  $\alpha_0$  is:

$$\alpha_s \left( \frac{s}{a} \right) = \alpha_0 + d_1(s) \alpha_0^2 + d_2(s) \alpha_0^3 + \dots, \quad (28)$$

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<sup>4</sup>The errors in the coefficients in eq. (25) (and following equations) are due to those in the numerical values of the integrals given in the appendix. They are typically 1 (or possibly 2) in the last digit, and are negligible in the evaluation of  $\overline{m}_b$ .



where

$$d_1(s) = -\frac{\beta_0}{2\pi} \ln(s) - \frac{\pi}{2N} + 2.13573N + N_f (-0.08413 + 0.0634 c_{\text{SW}} - 0.3750 c_{\text{SW}}^2) , \quad (29)$$

and  $\beta_0 = (11N - 2N_f)/3$ . The contribution to the right-hand side of eq. (29) for the gauge theory without fermions is found in ref. [10], and the quark contribution for Wilson fermions (i.e. with  $c_{\text{SW}} = 0$ ) can be obtained from ref. [11]. The coefficients of  $c_{\text{SW}}$  and  $c_{\text{SW}}^2$  are presented here for the first time. Although not needed for our present calculation, the two-loop coefficient in eq. (28),  $d_2(s)$ , for the pure-gauge theory can be found in ref. [12].

Combining eqs. (26) and (29) we obtain the result in eq. (12) for  $\delta m$  expressed in terms of the  $\overline{\text{MS}}$  coupling.

### 3.1 Numerical Results

The results for  $\mathcal{E}$  computed in lattice simulations to date, have been obtained in the quenched approximation. For the purposes of this study we take the results from the APE collaboration [13]:

$$a\mathcal{E} = 0.61(1) \quad \text{at } \beta = 6.0 \quad (a^{-1} = 2.0(2) \text{ GeV}) \quad (30)$$

$$a\mathcal{E} = 0.52(1) \quad \text{at } \beta = 6.2 \quad (a^{-1} = 2.9(3) \text{ GeV}) \quad (31)$$

$$a\mathcal{E} = 0.460(7) \quad \text{at } \beta = 6.4 \quad (a^{-1} = 3.8(3) \text{ GeV}) . \quad (32)$$

Of course the quenched calculation is incomplete and there is no procedure for determining  $\overline{m}_b$  from quenched computations of  $\mathcal{E}$  which is totally satisfactory. We will now describe our approach, but note that many readers may choose to follow different procedures, which are equally valid in the absence of unquenched results. We take the quenched results in eqs. (30)–(32) and determine the pole mass by combining them with the perturbative result for  $\delta m$  written in terms of the  $\overline{\text{MS}}$  coupling constant at the scale  $\overline{m}_b$  obtained using eqs. (28) and (29) with  $N_f = 0$ . We then derive  $\overline{m}_b$  from this value of the pole mass using continuum perturbation theory, eq. (11), but also with  $N_f = 0$ , to ensure the cancellation of renormalon singularities. We present the details and results in subsection 3.1.1.

In subsection 3.1.2 below we discuss the fermionic contributions in perturbation theory and demonstrate that they are large (of  $O(100)$  MeV or more for the lattice spacing considered in this paper). Finally in this section we compare our two-loop results with some standard procedures used to try to optimise the one-loop results, such as using the boosted coupling constant or a coupling defined at some average momentum for the process,  $q^*$ , (see subsection 3.1.3).

#### 3.1.1 Quenched Results for $\overline{m}_b$

In the quenched approximation we can rewrite  $\delta m$  in the form

$$a \delta m = 2.1173 \alpha_s(\overline{m}_b) + (3.707 \ln(\overline{m}_b a) - 1.306) \alpha_s^2(\overline{m}_b) . \quad (33)$$

$\beta$	$a^{-1}$ (GeV)	$\overline{m}_b$ (GeV) eq. (34)	$\overline{m}_b$ (GeV) eq. (35)
6.0	2.0(2)	4.37(5)	4.45(5)
6.2	2.9(3)	4.38(7)	4.47(7)
6.4	3.8(3)	4.38(7)	4.47(8)

Table 2: Values of  $\overline{m}_b$  obtained using eqs. (34) and (35).

Most of the very large coefficient 11.152 in the perturbation series written in terms of  $\alpha_0$  (see eq. (26)) has been absorbed into the coupling  $\alpha_s$ . This is frequently the case [14]. The implicit equation for  $\overline{m}_b$  is (see eq. (11))

$$\begin{aligned} \overline{m}_b = \Delta \left[ 1 + \frac{1}{\Delta a} \left\{ 2.1173 \alpha_s(\overline{m}_b) + (3.707 \ln(\overline{m}_b a) - 1.306) \alpha_s^2(\overline{m}_b) \right\} \right] \\ \times \left[ 1 - \frac{4}{3} \frac{\alpha_s(\overline{m}_b)}{\pi} - 11.66 \left( \frac{\alpha_s(\overline{m}_b)}{\pi} \right)^2 \right] \end{aligned} \quad (34)$$

where  $\Delta = m_B - \mathcal{E}$ . To the order we are working in, eq. (34) is equivalent to:

$$\begin{aligned} \overline{m}_b = \Delta \left[ 1 + \left\{ \frac{2.1173}{\Delta a} - 0.4244 \right\} \alpha_s(\overline{m}_b) \right. \\ \left. + \left\{ \frac{1}{\Delta a} (3.707 \ln(\overline{m}_b a) - 2.207) - 1.181 \right\} \alpha_s^2(\overline{m}_b) + \dots \right] . \end{aligned} \quad (35)$$

The difference of the results obtained using eqs. (34) and (35) will be an indication of the error due to 3-loop and higher order terms.

We estimate  $\overline{m}_b$  using equations (34) and (35). At this stage, in spite of using the quenched results for  $\mathcal{E}$ , we simply assume that the result is the physical one and for  $\alpha_s(\overline{m}_b)$  we take the coupling constant obtained from  $\alpha_s(M_Z) = 0.118(3)$  using the two-loop evolution equation with five flavours (this gives  $\alpha_s(\overline{m}_b) \simeq 0.22(1)$ ). Eqs. (34) and (35), which contain  $\overline{m}_b$  both on the left and right-hand sides, are solved by iteration and the corresponding results are presented in table 2. As mentioned above, the difference of the results obtained using eqs. (34) and (35) are due to our ignorance of three-loop and higher-order perturbative corrections. This difference is about 80–90 MeV. The results for different values of the lattice spacing are in remarkably good agreement. The errors on the values of  $\overline{m}_b$  in table 2 are due to the uncertainties in the values of the lattice spacing, in the values of  $\mathcal{E}$  and in  $\alpha_s(M_Z)$ . The dominant component in the errors is the first one, and is a consequence of the fact that using different physical quantities to determine the lattice spacing in quenched simulations, leads to differences of  $O(10\%)$  or so in the estimates of  $a$  (which correspond to differences of about 50 MeV in  $\overline{m}_b$ ). The errors in the results for  $\overline{m}_b$  in table 2 are strongly correlated and should not be combined in quadrature. For our best

$\beta$	$a^{-1}$ (GeV)	$\overline{m}_b$ (GeV) eq. (34)	$\overline{m}_b$ (GeV) eq. (35)
6.0	2.0(2)	4.52(4)	4.60(4)
6.2	2.9(3)	4.63(5)	4.75(5)
6.4	3.8(3)	4.78(6)	4.92(7)

Table 3: Values of  $\overline{m}_b$  obtained using eqs. (34) and (35) in each case dropping the terms which are explicitly of  $O(\alpha_s^2(\overline{m}_b))$ .

value we take the results at  $\beta = 6.0$  and quote:

$$\overline{m}_b = 4.41 \pm 0.05 \pm 0.10 \text{ GeV} . \quad (36)$$

The first error in eq. (36) is just that in table 2 and the second is an estimate of the uncertainty in higher order perturbative corrections, as manifested in the different values in the third and fourth columns of the table.

### 3.1.2 The Unquenched Calculation

We now briefly comment on the result including fermion loops. Consider eq. (12). In this case it is not true that most of the fermionic two-loop contribution is reabsorbed into the  $\overline{\text{MS}}$  coupling constant. The two-loop fermionic contribution is large, particularly with the improved action. Even with the tree-level improved action ( $c_{\text{SW}} = 1$ ) the fermionic two-loop contribution to  $\delta m$  varies from about 80 to about 150 MeV for lattice spacings in the range considered in this paper. For full  $O(a)$  improvement one expects  $c_{\text{SW}}$ , and hence the two-loop contributions, to be larger still. Since the fermionic contribution to  $\delta m$  is large, it is likely that unquenched results for  $\mathcal{E}$  will be significantly different from those in eqs. (30)–(32) for the corresponding values of the lattice spacing. Of course we are not yet in a position to check whether this expectation is true.

### 3.1.3 Comparison with the One-Loop Result for $\overline{m}_b$

In table 3 we present the results for  $\overline{m}_b$  obtained using one-loop perturbation theory in terms of  $\alpha_s(\overline{m}_b)$ . The errors in table 3 are also those due to the uncertainties in the values of the lattice spacings,  $\mathcal{E}$  and  $\alpha_s(M_Z)$ . Using this procedure, the variation of the results with  $\beta$  is relatively large and it is difficult to extract a meaningful result for  $\overline{m}_b$ .

In many calculations in which the perturbative matching factors are known only to one-loop order a different procedure is followed. Instead of using  $\alpha_s(\overline{m}_b)$  as the coupling constant in lattice perturbation theory, one uses  $\alpha_s(q^*)$  where  $q^*$  is an estimate of the “typical” loop momentum in the process [14]. We choose to define  $q^*$  by:

$$\log[(aq^*)^2] = \frac{1}{X} \int \frac{d^3k}{(2\pi)^3} \frac{\log[2A(k)]}{A(k)} , \quad (37)$$

where  $X$  and  $A(k)$  are defined in eqs. (A.1) and (A.2) respectively. With this definition  $q^*a = 1.446$ . Alternatively one might use a “boosted” lattice coupling constant [14]. In order to get an estimate of the precision and reliability of such procedures we define

$$\varepsilon(\delta m) = (\delta m)_{\text{two-loops}} - (\delta m)_{\text{one-loop}} , \quad (38)$$

where  $(\delta m)_{\text{two-loops}}$  is the two-loop result given in eq. (33) and  $(\delta m)_{\text{one-loop}}$  is the one-loop result obtained using one of the procedures described above. We find the following:

- i) The one-loop result  $\delta m = 2.1173 \alpha_s(q^*) a^{-1}$  reproduces the two-loop result in eq. (33) remarkably well when the  $\overline{\text{MS}}$  coupling constant is used. Specifically  $\varepsilon(\delta m) \simeq 10, 15$  and  $35 \text{ MeV}$  for  $\beta = 6.0, 6.2$  and  $6.4$  respectively.
- ii) The one-loop result varies significantly with the choice of “reasonable” coupling. For example, using the coupling defined from the inter-quark potential,  $\alpha_V(q^*)$ , one finds  $\varepsilon(\delta m) \simeq -210, -235$  and  $-315 \text{ MeV}$  for  $\beta = 6.0, 6.2$  and  $6.4$  respectively <sup>5</sup>.
- iii) The use of a boosted coupling constant,  $\tilde{\alpha}_s = \alpha_0/u_0^4$ , where  $\alpha_0$  is the lattice coupling and  $u_0$  is some estimate of the average value of the link-variable, underestimates the perturbative corrections significantly. For example, using the trace of the plaquette to define  $u_0$ ,  $\varepsilon(\delta m) \simeq 510, 610$  and  $670 \text{ MeV}$  for  $\beta = 6.0, 6.2$  and  $6.4$  respectively. This is the procedure which was used in ref. [15], and is the main reason for the low central quoted in that paper ( $\overline{m}_b = 4.15 \pm 0.05 \pm 0.20 \text{ GeV}$ ), where the error of  $200 \text{ MeV}$  was an estimate of the effects of higher orders in perturbation theory.

Thus we see that the range of one-loop perturbative results for  $\delta m$ , and hence for  $\overline{m}_b$  is very large; indeed it is considerably larger than the precision required for the lattice results for the quark mass to be phenomenologically interesting. This is the main motivation for the two-loop calculation presented in this paper.

It should also be noted that the two-loop result in the (continuum) perturbation series relating  $m_b^{\text{pole}}$  and  $\overline{m}_b$  is also large (changing the result for  $\overline{m}_b$  by  $O(250 \text{ MeV})$ ). Resummation techniques can also be used to try to improve the convergence of this series (see for example refs. [16] and references therein).

## 4 Conclusions

The mass of the  $b$ -quark is one of the fundamental parameters of the standard model of particle physics. It can be determined from lattice simulations of the HQET, by computing the time behaviour of hadronic correlation functions. An ingredient of such a determination of  $\overline{m}_b$ , is the perturbation series for  $\delta m$ , the mass generated in the lattice formulation of the HQET. In this paper we have evaluated the two-loop term in the lattice perturbation

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<sup>5</sup>For the numerical value of  $\alpha_V(q^*)$  we take  $\alpha_V(q^*) = \alpha_s(q^*)(1 + 0.822 \alpha_s(q^*))$ , and use the physical value of the  $\overline{\text{MS}}$  coupling  $\alpha_s(q^*)$  obtained by evolving the result  $\alpha_s(M_Z) = 0.118(3)$  using the two-loop renormalisation group equation.

series for  $\delta m$ , and the result is presented in eq. (26). Combining our result for  $\delta m$  with the values of  $\mathcal{E}$  obtained by the APE collaboration, we obtain the result for  $\overline{m}_b$ , given in eq. (1).

We would like to determine  $\overline{m}_b$  with a precision better than  $O(\Lambda_{\text{QCD}})$ . This is an example of a calculation of a power correction (at leading order we can use the mass of the pseudoscalar meson to estimate the quark mass). As with any power correction, to achieve the required precision is very difficult [7]. We have argued in section 3.1.3 that, using one-loop matching, the uncertainty in the determination of  $\overline{m}_b$  is several hundred MeV. Our estimate (which in reality can only be an educated “guesstimate”) of the uncertainty in  $\overline{m}_b$  after the two-loop effects are included is that it is of  $O(100 \text{ MeV})$ .

We consider the question of the precision which can be reached when only using one-loop matching to be so important that we repeat here part of the discussion of section 3.1.3. At one-loop level we have

$$\delta m = 2.1173 \alpha_s a^{-1} . \quad (39)$$

As an example let us consider the simulation at  $\beta = 6.0$  (for which  $a^{-1} = 2.0(2) \text{ GeV}$ ). Now as “reasonable” choices of  $\alpha_s$  we take <sup>6</sup>:

- i) the  $\overline{\text{MS}}$  coupling at  $q^*$ ,  $\alpha_s(q^*) \simeq 0.253$ , so that  $\delta m \simeq 1.07 \text{ GeV}$ .
- ii) the coupling in the “potential”-scheme at  $q^*$ ,  $\alpha_V(q^*) = 0.306$ , so that  $\delta m \simeq 1.29 \text{ GeV}$ .
- iii) the “boosted” coupling, defined by  $\alpha_0/u_0^4 \simeq 0.134$ , where  $u_0$  is an estimate of the average link-variable, obtained from the fourth root of the plaquette. With this boosted coupling  $\delta m \simeq 0.57 \text{ GeV}$ .

Since the perturbative coefficient is relatively large (2.1173 rather than  $1/\pi$  say) and  $a^{-1} \gg \Lambda_{\text{QCD}}$ , the spread of results obtained using reasonable choices for the expansion parameter  $\alpha_s$  is several hundred MeV. It is, therefore, not possible to achieve a precision in  $\delta m$  (and hence in  $\overline{m}_b$ ) which is better than  $O(\Lambda_{\text{QCD}})$  without calculating the two-loop (or even higher order) matching coefficients. This is an example of a generic problem in the evaluation of power corrections, and is also not restricted to lattice computations.

It should be said that our view that the ignorance of higher order perturbative coefficients implies that the uncertainties in the results for power corrections to physical quantities are large is not universally accepted. In this paper we have confirmed our view with a specific two-loop calculation. For  $m_b$  the leading correction is linear, and correspondingly we have had to subtract the linear divergence (i.e. the terms which diverged linearly in  $1/a$ ) in  $\mathcal{E}$  using perturbation theory. In other important examples one needs to subtract quadratic or even higher order divergences and the difficulty to achieve the required precision increases enormously.

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<sup>6</sup>In the following examples we take the central value  $a^{-1} = 2 \text{ GeV}$ . There is a 10% error associated with the uncertainty in the scale, but as we wish to study the variation with the choice of coupling constant, we keep a fixed value of  $a$ .

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## A Appendix: Two-Loop Contribution to Large Wilson Loops

Our calculation of  $\delta m$  is based on the fact that it is proportional to the logarithm of the perimeter term in the perturbative expansion of large Wilson loops. In this appendix we present the details of the evaluation of the two-loop contribution to large Wilson loops.

The appendix is organised as follows. In the opening section we define the multidimensional integrals which appear in our result for  $W_4$  and present their numerical values. A description of the evaluation of the terms in  $W_4$  which grow at least linearly with  $R$  and  $T$  in the pure gauge-theory (i.e. in the theory without light quarks) is presented in section A.2. The fermionic contributions to  $W_4$  are evaluated in section A.3.

### A.1 Integrals

The two-loop contribution to  $\delta m$  will be presented in terms of a number of multidimensional integrals,  $X, L, Y, W, V_{1,2}, V_W$  and  $V_{SW}$ , which have to be evaluated numerically. In this subsection we define these integrals and present their values. All the integrals have limits of integration from  $-\pi$  to  $\pi$  for each momentum component.

1. The first three integrals are one-loop ones. In each case it is straightforward to perform the integral over one component of momentum analytically, leaving a three-dimensional integral to be performed numerically. The first of these is

$$X \equiv \int \frac{d^3 k}{(2\pi)^3} \frac{1}{A(k)} = 0.50546 \quad (\text{A.1})$$

where

$$A(k) = \sum_{i=1}^3 (1 - \cos(k_i)) . \quad (\text{A.2})$$

$X$  is the integral which contributes to the one-loop component of  $\delta m$ .

2. The second one-loop integral is

$$L \equiv \int \frac{d^3 k}{(2\pi)^3} \frac{1}{\sqrt{(1 + A(k))^2 - 1}} = 0.30987 . \quad (\text{A.3})$$

3. The third integral arises in the calculation of the wave-function renormalisation at one-loop level:

$$Y(T) \equiv \int \frac{d^3 k}{(2\pi)^3} \frac{1}{A \sqrt{(1 + A)^2 - 1}} (1 - \beta^T), \quad (\text{A.4})$$

where

$$\beta = 1 + A - \sqrt{(1 + A)^2 - 1} , \quad (\text{A.5})$$

and  $A$  and  $\beta$  are implicitly functions of  $k$ . Without the  $\beta^T$  term on the right-hand side of eq. (A.4) the integral would be divergent (it depends logarithmically on  $T$ ). In the final result for  $\delta m$ , any dependence on  $Y(T)$  or  $Y(R)$  must cancel.

4. The remaining integrals are 7-dimensional and for these the results are generally obtained with poorer relative precision. The first of these is

$$W \equiv \int \frac{d^3 k}{(2\pi)^3} \frac{1}{A(k)} \int \frac{d^3 p}{(2\pi)^3} \frac{1}{A(p)} \cdot \int \frac{dq}{2\pi} \frac{\sin^2(q)}{(4 \sin^2(q/2) + 2A(k))(4 \sin^2(q/2) + 2A(p))} = 1.313(3) \cdot 10^{-2} . \quad (\text{A.6})$$

5. There are two integrals which arise from the gluonic contribution to the vacuum-polarisation. The first of these is

$$V_1 \equiv \int \frac{d^3 p}{(2\pi)^3} \frac{d^4 k}{(2\pi)^4} \frac{(1 + \cos(k_\mu))}{A^2(p)(4 - C_4(k))} \left\{ \frac{4 - C_4(2p + k)}{4 - C_4(p + k)} - 1 \right\} \\ = 7.008(5) \cdot 10^{-2} , \quad (\text{A.7})$$

where  $p_\mu = 0$  ( $\mu$  is a fixed direction and the integral over  $p$  is over the 3 components other than the  $\mu$ -component). The function  $C_4$  is defined by

$$C_4(r) \equiv \sum_{\lambda=1}^4 \cos(r_\lambda) . \quad (\text{A.8})$$

6. The second integral arising from the gluonic vacuum-polarisation graphs is

$$V_2 \equiv \int \frac{d^3 p}{(2\pi)^3} \frac{d^4 k}{(2\pi)^4} \frac{\sin^2(k_\mu)}{A^2(p)(4 - C_4(k))} \left\{ \frac{1 + \sum_{i \neq \mu} \cos(p_i)}{2(4 - C_4(p + k))} - \frac{2}{4 - C_4(k)} \right\} \\ = -2.130(1) \cdot 10^{-2} , \quad (\text{A.9})$$

where, again,  $\mu$  is a fixed direction and  $p_\mu = 0$ .

7. The final two integrals correspond to graphs containing fermionic contributions to the vacuum-polarisation. For Wilson-fermions the relevant integral is

$$V_W \equiv \int \frac{d^3 p}{(2\pi)^3} \frac{d^4 k}{(2\pi)^4} \frac{1}{A^2(p)} \frac{1}{S(k)} \left[ \frac{Z_W(p, k)}{S(q)} - \frac{Z_W(p = 0, k)}{S(k)} \right] , \quad (\text{A.10})$$



where  $q \equiv p + k$ ,  $p_\mu = 0$ ,

$$S(k) = \sum_{\lambda=1}^4 \sin^2(k_\lambda) + W^2(k) , \quad (\text{A.11})$$

$$W(k) = 2 \sum_{\lambda=1}^4 \sin^2\left(\frac{k_\lambda}{2}\right) , \quad (\text{A.12})$$

and

$$\begin{aligned} Z_W(p, k) = & -8 \cos^2(k_\mu) \sin^2(k_\mu) + 4 \sum_{\lambda=1}^4 \sin(k_\lambda) \sin(q_\lambda) \\ & + 4 \cos(2k_\mu) W(k) W(q) - 8 \cos(k_\mu) \sin^2(k_\mu) [W(k) + W(q)] . \end{aligned} \quad (\text{A.13})$$

$W(k)$ , the Wilson term in the fermion propagator defined in eq. (A.12), should not be confused with the integral  $W$  defined in eq. (A.6). We find that

$$V_W = -2.145(1) \cdot 10^{-2} . \quad (\text{A.14})$$

8. Finally we present the integral,  $V_{\text{SW}}$  required to evaluate the additional fermionic contributions when the SW-improved action is used,

$$V_{\text{SW}} \equiv \int \frac{d^3 p}{(2\pi)^3} \frac{d^4 k}{(2\pi)^4} \frac{1}{A^2(p)} \frac{Z_{\text{SW}}}{S(k)S(q)} , \quad (\text{A.15})$$

where, again,  $q = p + k$ ,  $p_\mu = 0$  and

$$\begin{aligned} Z_{\text{SW}} = & c_{\text{SW}} \left\{ 4 \sin^2(k_\mu) \sum_{\lambda=1}^4 \sin(p_\lambda) [\sin(q_\lambda) - \sin(k_\lambda)] \right. \\ & \left. - 4 \cos(k_\mu) \left( W(k) \sum_{\lambda=1}^4 \sin(p_\lambda) \sin(q_\lambda) - W(q) \sum_{\lambda=1}^4 \sin(p_\lambda) \sin(k_\lambda) \right) \right\} \\ & - c_{\text{SW}}^2 \left\{ \left( 2 \sin^2(k_\mu) - \sum_{\lambda=1}^4 \sin(q_\lambda) \sin(k_\lambda) + W(k) W(q) \right) \sum_{\rho=1}^3 \sin^2(p_\rho) \right. \\ & \left. + 2 \sum_{\lambda=1}^4 \sin(p_\lambda) \sin(k_\lambda) \sum_{\sigma=1}^4 \sin(p_\sigma) \sin(q_\sigma) \right\} . \end{aligned} \quad (\text{A.16})$$

Evaluating the integrals numerically we find

$$V_{\text{SW}} = 2.63(2) \cdot 10^{-3} c_{\text{SW}} - 2.974(1) \cdot 10^{-2} c_{\text{SW}}^2 . \quad (\text{A.17})$$

## A.2 The Gluonic Contribution to $W_4(\mathbf{R}, \mathbf{T})$

In this section we outline the evaluation of the gluonic contribution to the two-loop term in the Wilson loop,  $-g^4 W_4(R, T)$ . Following ref. [8], we distinguish 5 contributions to  $W_4$ <sup>7</sup>:

$$W_4(R, T) = W_{S_1} + W_I + W_{II} + W_{VP} + \overline{W}_{VP} . \quad (\text{A.18})$$

We now evaluate each of these in turn, picking up the contributions which grow as  $R$ ,  $T$ ,  $R^2$ ,  $T^2$  or  $RT$ .

**$W_{S_1}$ :** This contribution comes from the “spider” graph and is given in eq. (3.6) of ref. [8]. It is proportional to

$$\begin{aligned} & \int \frac{d^4 k}{(2\pi)^4} \frac{d^4 p}{(2\pi)^4} \frac{1}{D(p)D(k)D(p+k)} \left[ \left\{ \frac{\sin^2(\frac{1}{2}p_\mu R)}{\sin(\frac{1}{2}p_\mu)} \sin(\frac{1}{2}p_\nu T) \cos(\frac{1}{2}p_\nu) \sin(\frac{1}{2}(2k+p)_\mu) \right. \right. \\ & \quad \times \left[ \frac{\sin(\frac{1}{2}p_\nu T) \sin(\frac{1}{2}(2k+p)_\nu)}{\sin(\frac{1}{2}p_\nu) \sin(\frac{1}{2}k_\nu) \sin(\frac{1}{2}(p+k)_\nu)} - \frac{\sin(\frac{1}{2}(2k+p)_\nu T)}{\sin(\frac{1}{2}k_\nu) \sin(\frac{1}{2}(p+k)_\nu)} \right] \\ & \quad + 4 \frac{\sin(\frac{1}{2}p_\mu R)}{\sin(\frac{1}{2}p_\mu)} \frac{\sin(\frac{1}{2}k_\mu R)}{\sin(\frac{1}{2}k_\mu)} \frac{\sin(\frac{1}{2}(p+k)_\nu T)}{\sin(\frac{1}{2}(p+k)_\nu)} \sin(\frac{1}{2}p_\nu T) \cos(\frac{1}{2}k_\nu T) \\ & \quad \left. \left. \times \cos(\frac{1}{2}(p+k)_\mu R) \cos(\frac{1}{2}(p+k)_\mu) \sin(\frac{1}{2}((k-p)_\nu)) \right\} + \{(\mu, R) \leftrightarrow (\nu, T)\} \right] , \quad (\text{A.19}) \end{aligned}$$

where  $D(p)$  is defined in eq. (17). By detailed inspection of the infrared behaviour of the integral, one can see that there is insufficient enhancement from the denominators to give a term proportional to  $R$  or  $T$ . Thus there is no contribution to  $\delta m$  from  $W_{S_1}$ .

**$W_I$ :**  $W_I$  is defined to be the “expectation value of the non-abelian part of the order  $g^4$  term in the expansion of the Wilson loop” [8]. It is presented in eq. (3.7) of ref. [8] and contains several terms which we consider in turn. The first five contributions,  $T_1$ – $T_5$ , are products of the one-loop integrals defined in section A.1 and are hence relatively straightforward to evaluate. We therefore simply define these contributions and present the corresponding results in terms of the integrals  $X$ ,  $L$ , and  $Y$ .

$$\begin{aligned} T_1 &= -\frac{(N^2 - 1)}{3} \Delta_0 \left[ \left\{ \int \frac{d^4 p}{(2\pi)^4} \frac{\sin^2(\frac{1}{2}p_\nu T)}{D(p)} \left( \frac{\sin^2(\frac{1}{2}p_\mu R)}{\sin^2(\frac{1}{2}p_\mu)} + \frac{1}{2} \frac{\sin(\frac{1}{2}p_\mu R) \sin(\frac{1}{2}p_\mu (R-2))}{\sin^2(\frac{1}{2}p_\mu)} \right) \right\} \right. \\ & \quad \left. + \{(\mu, R) \leftrightarrow (\nu, T)\} \right] \quad (\text{A.20}) \end{aligned}$$

$$= -\frac{(N^2 - 1)}{16} (R + T) X L . \quad (\text{A.21})$$

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<sup>7</sup>The five contributions in eq. (A.18) are defined explicitly in eqs. (3.6)–(3.10) of ref. [8].

In eq. (A.20)

$$\Delta_0 = \int \frac{d^4 k}{(2\pi)^4} \frac{1}{D(k)} = \frac{L}{2} . \quad (\text{A.22})$$

We repeat that we only keep terms which grow at least linearly with  $R$  and  $T$ .

$$\begin{aligned} T_2 = & -\frac{(N^2 - 1)}{2} \left[ \left\{ \int \frac{d^4 k}{(2\pi)^4} \frac{1}{D(k)} \left( \frac{\sin^2(\frac{1}{2}k_\nu T)}{\sin^2(\frac{1}{2}k_\nu)} + \frac{1}{6} \frac{\sin^2(\frac{1}{2}k_\mu R)}{\sin^2(\frac{1}{2}k_\mu)} \right) \right. \right. \\ & \times \left. \int \frac{d^4 p}{(2\pi)^4} \frac{\sin^2(\frac{1}{2}p_\nu T)}{D(p)} \frac{\sin^2(\frac{1}{2}p_\mu R)}{\sin^2(\frac{1}{2}p_\mu)} \right\} + \{(\mu, R) \leftrightarrow (\nu, T)\} \Big] \quad (\text{A.23}) \end{aligned}$$

$$\begin{aligned} \simeq & -\frac{(N^2 - 1)}{8} [XT - Y(T)] [XR - Y(R)] - \\ & \frac{(N^2 - 1)}{96} [XR - Y(R)]^2 - \frac{(N^2 - 1)}{96} [XT - Y(T)]^2 . \quad (\text{A.24}) \end{aligned}$$

$$T_3 = \frac{(N^2 - 1)}{12} \left[ \left\{ \left[ \int \frac{d^4 p}{(2\pi)^4} \frac{\sin^2(\frac{1}{2}p_\nu T)}{D(p)} \frac{\sin^2(\frac{1}{2}p_\mu R)}{\sin^2(\frac{1}{2}p_\mu)} \right]^2 \right\} + \{(\mu, R) \leftrightarrow (\nu, T)\} \right] \quad (\text{A.25})$$

$$\simeq \frac{N^2 - 1}{192} \{ [XR - Y(R)]^2 + [XT - Y(T)]^2 \} . \quad (\text{A.26})$$

$$\begin{aligned} T_4 = & \frac{2(N^2 - 1)}{3} \int \frac{d^4 k}{(2\pi)^4} \frac{\sin^2(\frac{1}{2}k_\nu T)}{D(k)} \frac{\sin^2(\frac{1}{2}k_\mu R)}{\sin^2(\frac{1}{2}k_\mu)} \\ & \times \int \frac{d^4 p}{(2\pi)^4} \frac{\sin^2(\frac{1}{2}p_\mu R)}{D(p)} \frac{\sin^2(\frac{1}{2}p_\nu T)}{\sin^2(\frac{1}{2}p_\nu)} \quad (\text{A.27}) \end{aligned}$$

$$\simeq \frac{(N^2 - 1)}{24} (XR - Y(R)) (XT - Y(T)) . \quad (\text{A.28})$$

$$T_5 = \frac{(N^2 - 1)}{4} \int \frac{d^4 k}{(2\pi)^4} \frac{\sin^2(\frac{1}{2}k_\mu R)}{D(k)} \int \frac{d^4 p}{(2\pi)^4} \frac{\sin^2(\frac{1}{2}p_\nu T)}{D(p)} \quad (\text{A.29})$$

$$\simeq \frac{(N^2 - 1)}{16} (XR - Y(R)) (XT - Y(T)) . \quad (\text{A.30})$$

The remaining three terms contain nested integrals and are considerably more compli-

cated to evaluate. The first of these is

$$T_6 = \frac{(N^2 - 1)}{32} \iint \frac{d^4 k}{(2\pi)^4} \frac{d^4 p}{(2\pi)^4} \frac{1}{D(p)D(k)} \left[ \left[ \frac{\sin(\frac{1}{2}(p+k)_\mu R) \sin(\frac{1}{2}(p-k)_\mu) - \sin(\frac{1}{2}(p-k)_\mu R) \sin(\frac{1}{2}(p+k)_\mu)}{\sin(\frac{1}{2}(p+k)_\mu)} \right]^2 \times \frac{\sin^2(\frac{1}{2}(p+k)_\nu T)}{\sin^2(\frac{1}{2}p_\mu) \sin^2(\frac{1}{2}k_\mu)} \right] + \{(\mu, R) \leftrightarrow (\nu, T)\} \right] . \quad (\text{A.31})$$

In order to extract the behaviour of this integral at large  $R$  and  $T$  consider the following two-dimensional integral

$$I = \int \frac{dk_\mu}{2\pi} \frac{dp_\mu}{2\pi} \frac{1}{D(p)D(k)} \frac{N}{4 \sin^2(p_\mu/2) 4 \sin^2(k_\mu/2) 4 \sin^2((p+k)_\mu/2)} , \quad (\text{A.32})$$

where

$$N = \left[ 4 \sin \left( \frac{(p+k)_\mu R}{2} \right) \sin \left( \frac{(p-k)_\mu}{2} \right) - 4 \sin \left( \frac{(p-k)_\mu R}{2} \right) \sin \left( \frac{(p+k)_\mu}{2} \right) \right]^2 . \quad (\text{A.33})$$

It is convenient to use partial fractions to simplify I:

$$I = I_1 - (I_2 + I_3) + I_4 , \quad (\text{A.34})$$

where

$$\begin{aligned} I_1 &= \frac{1}{4A(p)A(k)} \int \frac{dp_\mu}{2\pi} \frac{dk_\mu}{2\pi} \frac{N}{4 \sin^2(p_\mu/2) 4 \sin^2(k_\mu/2) 4 \sin^2((p+k)_\mu/2)} \\ I_2 &= \frac{1}{4A(p)A(k)} \int \frac{dp_\mu}{2\pi} \frac{dk_\mu}{2\pi} \frac{N}{4 \sin^2(p_\mu/2) (4 \sin^2(k_\mu/2) + 2A(k)) 4 \sin^2((p+k)_\mu/2)} \\ I_3 &= \frac{1}{4A(p)A(k)} \int \frac{dp_\mu}{2\pi} \frac{dk_\mu}{2\pi} \frac{N}{(4 \sin^2(p_\mu/2) + 2A(p)) 4 \sin^2(k_\mu/2) 4 \sin^2((p+k)_\mu/2)} \\ I_4 &= \frac{1}{4A(p)A(k)} \int \frac{dp_\mu}{2\pi} \frac{dk_\mu}{2\pi} \frac{N}{4 \sin^2((p+k)_\mu/2)} \\ &\quad \times \frac{1}{(4 \sin^2(p_\mu/2) + 2A(p)) (4 \sin^2(k_\mu/2) + 2A(k))} . \end{aligned}$$

$A(p)$  and  $A(k)$  are defined in eq. (A.2), where the sum is over the three components of  $p$  and  $k$  other than the  $\mu$ -component.

$I_1$ – $I_4$  can be evaluated by changing integration variables to  $z = \exp(ip_\mu)$  and  $\omega = \exp(i(p+k)_\mu)$  and using Cauchy's contour integration theory. In terms of these complex variables

$$N = \omega^{-(R+1)} [(1+z)(\omega^R - 1)(1 - \omega/z) - (\omega - 1)(z^R + 1)(1 - (\omega/z)^R)]^2 . \quad (\text{A.35})$$

In this way we obtain

$$\begin{aligned}
I_1 &= \frac{R(R-1)}{4} X^2 \\
I_2 &= \frac{3R}{4} XY(R) - \frac{R}{4} X^2 + \frac{R}{4} XL \\
I_3 &= I_2 \\
I_4 &= RW .
\end{aligned}$$

Note that

$$\int \frac{dp_\mu}{2\pi} \frac{dk_\mu}{2\pi} \frac{N}{64 \sin^2(p_\mu/2) \sin^2(k_\mu/2) \sin^2((p+k)_\mu/2)} = R(R-1) . \quad (\text{A.36})$$

Since we are only interested in identifying the terms which grow at least linearly with  $R$  or  $T$ , we can replace  $\sin^2(\frac{1}{2}(p+k)_\nu T)$  in eq. (A.31) with the factor  $\frac{1}{2}$ , thus obtaining

$$T_6 = \frac{N^2 - 1}{16} \left[ \frac{R(R+1)}{4} X^2 - \frac{3R}{2} XY(R) - \frac{R}{2} XL + RW \right] + R \leftrightarrow T . \quad (\text{A.37})$$

The second nested integral is

$$\begin{aligned}
T_7 &= \frac{N^2 - 1}{6} \iint \frac{d^4 k}{(2\pi)^4} \frac{d^4 p}{(2\pi)^4} \frac{1}{D(p)D(k)} \\
&\quad \left[ \left\{ \sin^2(\tfrac{1}{2}p_\nu T) \frac{\sin(\tfrac{1}{2}p_\mu R)}{\sin(\tfrac{1}{2}p_\mu)} \frac{\sin(\tfrac{1}{2}k_\mu R)}{\sin(\tfrac{1}{2}k_\mu)} \frac{\sin(\tfrac{1}{2}(p+k)_\mu R)}{\sin(\tfrac{1}{2}(p+k)_\mu)} \right\} + \{(\mu, R) \leftrightarrow (\nu, T)\} \right] . \quad (\text{A.38})
\end{aligned}$$

Using the fact that

$$\int \frac{dp_\mu}{2\pi} \int \frac{dk_\mu}{2\pi} \frac{\sin(p_\mu R/2) \sin(k_\mu R/2) \sin((p+k)_\mu R/2)}{\sin(p_\mu/2) \sin(k_\mu/2) \sin((p+k)_\mu/2)} = R , \quad (\text{A.39})$$

we readily obtain

$$T_7 = \frac{N^2 - 1}{48} X^2 (R + T) . \quad (\text{A.40})$$

The final contribution to  $W_I$  is

$$\begin{aligned}
T_8 = & -\frac{(N^2-1)}{6} \iint \frac{d^4k}{(2\pi)^4} \frac{d^4p}{(2\pi)^4} \frac{1}{D(p)D(k)} \\
& \left[ \left\{ \sin^2(\tfrac{1}{2}p_\nu T) \frac{\sin(\tfrac{1}{2}p_\mu R)}{\sin(\tfrac{1}{2}p_\mu)} \left[ \frac{\sin(\tfrac{1}{2}p_\mu(R-2)) \cos((p+k)_\mu)}{\sin(\tfrac{1}{2}p_\mu) \sin^2(\tfrac{1}{2}k_\mu)} \right. \right. \right. \\
& - \frac{\sin(\tfrac{1}{2}(p+k)_\mu(R-2)) \cos(\tfrac{1}{2}k_\mu(R+1)+p_\mu)}{\sin(\tfrac{1}{2}(p+k)_\mu) \sin^2(\tfrac{1}{2}k_\mu)} + \frac{\sin(\tfrac{1}{2}p_\mu(R-2)) \cos(\tfrac{1}{2}p_\mu - k_\mu)}{\sin(\tfrac{1}{2}p_\mu) \sin(\tfrac{1}{2}k_\mu) \sin(\tfrac{1}{2}(p+k)_\mu)} \\
& - \frac{\sin(\tfrac{1}{2}k_\mu(R-2)) \cos(\tfrac{1}{2}(p+k)_\mu R + \tfrac{1}{2}k_\mu - p_\mu)}{\sin(\tfrac{1}{2}(p+k)_\mu) \sin^2(\tfrac{1}{2}k_\mu)} \\
& + \frac{\sin(\tfrac{1}{2}(p+k)_\mu(R-2)) \cos(\tfrac{1}{2}k_\mu(R+2) + \tfrac{1}{2}p_\mu)}{\sin(\tfrac{1}{2}k_\mu) \sin(\tfrac{1}{2}p_\mu) \sin(\tfrac{1}{2}(p+k)_\mu)} \\
& \left. \left. - \frac{\sin(\tfrac{1}{2}k_\mu(R-2)) \cos(\tfrac{1}{2}(p-k)_\mu R - k_\mu - p_\mu)}{\sin(\tfrac{1}{2}p_\mu) \sin^2(\tfrac{1}{2}k_\mu)} \right] \right\} + \{(\mu, R) \leftrightarrow (\nu, T)\} \Big] , \quad (\text{A.41})
\end{aligned}$$

for which, by using partial fractions as in the evaluation of  $T_6$ , we find

$$T_8 = \frac{(N^2-1)}{48} X [-XR^2 - XR + 5Y(R)R + 4LR] + R \leftrightarrow T . \quad (\text{A.42})$$

Summing up the terms  $T_1$  to  $T_8$  to obtain  $W_I$  we find

$$\begin{aligned}
W_I = & \sum_{i=1}^8 T_i = -\frac{(N^2-1)}{48} (XR - Y(R))(XT - Y(T)) \\
& - \frac{(N^2-1)}{192} \{ (XR - Y(R))^2 + (XT - Y(T))^2 \} \\
& + \frac{(N^2-1)}{192} \{ -R^2 X^2 + 3RX^2 + 2XY(R)R - 2RXL + 12RW + R \leftrightarrow T \} . \quad (\text{A.43})
\end{aligned}$$

**W<sub>II</sub>:**  $W_{II}$  is the “abelian part of the expansion of order  $g^4$ ”, and is defined in eq. (3.8) of ref. [8]. It is very straightforward to evaluate:

$$W_{II} = -\frac{(2N^2-3)(N^2-1)}{6N^2} [\overline{W}_2(R, T)]^2 \quad (\text{A.44})$$

$$= -\frac{(2N^2-3)(N^2-1)}{96N^2} [X(R+T) - Y(R) - Y(T)]^2 , \quad (\text{A.45})$$

where  $\overline{W}_2$  has been defined in eq. (18).

**W<sub>VP</sub>:**  $W_{VP}$  is part of the contribution to the diagrams containing gluonic contributions to the vacuum polarisation, and is defined in eq.(3.9) of ref. [8]. It can be written in the form:

$$W_{VP} = \frac{(N^2 - 1)}{N} \frac{(R + T)}{8} \int \frac{d^3 p}{(2\pi)^3} \left( \frac{\Pi_{\mu\mu}^a(p; p_\mu = 0) - \Pi_{\mu\mu}^a(p = 0)}{A^2(p)} \right), \quad (\text{A.46})$$

where there is no implied sum over  $\mu$ , and

$$\begin{aligned} \Pi_{\mu\mu}^a(p; p_\mu = 0) &= \frac{N}{6} \left( \frac{7L}{2} - \frac{5}{8} \right) A(p) + \\ N \int \frac{d^4 k}{(2\pi)^4} \frac{1}{D(p+k)D(k)} &\left\{ (1 + \cos(k_\mu))(4 - C_4(2p+k)) + \sin^2(k_\mu) \left( 1 + \sum_{i \neq \mu} \cos(p_i) \right) \right\}. \end{aligned} \quad (\text{A.47})$$

Although  $\Pi_{\mu\mu}^a(p = 0) = 0$ , it is nevertheless convenient to subtract it (in the form of eq. (A.47) with  $p = 0$ ) in the numerator of the integrand in eq. (A.46) and to write  $W_{VP}$  in terms of the integrals  $V_1$  and  $V_2$  defined in eqs. (A.7) and (A.9). This subtraction introduces non-zero contributions to each of  $V_1$  and  $V_2$ , rendering these integrals convergent, but of course these contributions cancel in  $W_{VP}$ . In this way we obtain

$$W_{VP} = \frac{(N^2 - 1)}{32} (R + T) (V_1 + 2V_2) + \frac{(N^2 - 1)}{48} (R + T) \left( \frac{7L}{2} - \frac{5}{8} \right) X. \quad (\text{A.48})$$

**$\overline{W}_{VP}$ :**  $\overline{W}_{VP}$ , the remaining contribution to the diagrams containing gluonic contributions to the vacuum polarisation [8] is defined in eq. (3.10) of ref. [8] and is simple to evaluate:

$$\overline{W}_{VP} = \frac{(2N^2 - 3)(N^2 - 1)}{96N^2} [(R + T)X - Y(R) - Y(T)]. \quad (\text{A.49})$$

### A.2.1 Total Gluonic Contribution to $W_4$ :

Summing up the contributions from eqs. (A.43), (A.45), (A.48) and (A.49), and keeping only those terms which grow at least linearly with  $R$  and  $T$ , we obtain for the total gluonic contribution to  $W_4$ :

$$\begin{aligned} W_4^{\text{gluon}} &= -\frac{(N^2 - 1)^2}{32N^2} X^2 (R + T)^2 + \frac{(N^2 - 1)^2}{16N^2} X(R + T)(Y(R) + Y(T)) \\ &\quad + \frac{(N^2 - 1)}{192} \{3X^2 - 2XL + 12W\} (R + T) \\ &\quad + \frac{(N^2 - 1)}{96} \left\{ 3V_1 + 6V_2 + 7LX - \frac{5}{4}X \right\} (R + T) + \frac{(N^2 - 1)(2N^2 - 3)}{96N^2} X(R + T). \end{aligned} \quad (\text{A.50})$$

### A.3 Evaluation of the Fermionic Contribution to $W_4(\mathbf{R}, \mathbf{T})$

In this section we evaluate the diagrams containing fermionic contributions to the vacuum polarisation. This contribution is also given by eq. (A.46) but with  $\Pi_{\mu\mu}^a \rightarrow \Pi_{\mu\mu}^{\text{fermion}}$ , where  $\Pi_{\mu\mu}^{\text{fermion}}$  is the fermionic contribution to the vacuum polarisation graph:

$$\Pi_{\mu\mu}^{\text{fermion}}(p; p_\mu = 0) = \frac{N_f}{2} \int \frac{d^4k}{(2\pi)^4} \frac{Z_W(p, k) + Z_{\text{SW}}(p, k)}{S(k)S(q)} , \quad (\text{A.51})$$

where  $q = p + k$ ,  $S(k)$  is defined in eq. (A.11) and  $Z_{W,\text{SW}}(p, k)$  are defined in eqs. (A.13) and (A.16) respectively.  $N_f$  is the number of active light-quark flavours and we distinguish between the terms from the Wilson Fermion action (labelled by w) and the additional terms in the improved action with coefficient  $c_{\text{SW}}$  (labelled by sw). Thus the fermionic contribution to  $W_4$  is

$$W_4^{\text{fermion}} = \frac{(N^2 - 1)N_f}{16N} (R + T) (V_W + V_{\text{SW}}) . \quad (\text{A.52})$$